BIT Numerical Mathematics **??:** ??–??, 2006.

LINEARLY IMPLICIT TIME STEPPING METHODS FOR NUMERICAL WEATHER PREDICTION

SEBASTIAN REICH

Institut für Mathematik, Universität Potsdam, Postfach 60 15 53, D-14415 Potsdam, Germany. email: sreich@math.uni-potsdam.de

This paper is dedicated to the memory of Germund Dahlquist.

Abstract.

The efficient time integration of the dynamic core equations for numerical weather prediction (NWP) remains a key challenge. One of the most popular methods is currently provided by implementations of the semi-implicit semi-Lagrangian (SISL) method, originally proposed by Robert [5]. Practical implementations of the SISL method are, however, not without certain shortcomings with regard to accuracy, conservation properties and stability. Based on recent work by Gottwald, Frank & Reich [2], Frank, Reich, Staniforth, White & Wood [3] and Wood, Staniforth & Reich [9] we propose an alternative semi-Lagrangian implementation based on a set of regularized equations and the popular Störmer-Verlet time stepping method in the context of the shallow-water equations (SWEs). Ultimately, the goal is to develop practical implementations for the 3D Euler equations that overcome some or all shortcomings of current SISL implementations.

AMS subject classification: 65M12, 65M99, 65L20, 65L06, 86A10

Key words: numerical weather prediction, linearly implicit time stepping methods, semi-Lagrangian method, Störmer-Verlet method, shallow-water equations

1 Introduction

Germund Dahlquist's work has significantly contributed to our understanding of numerical time stepping methods and their stability properties. This paper, devoted to the memory of Germund Dahlquist, summarizes and further develops recent results concerning linearly implicit time stepping methods for numerical weather prediction (NWP).

NWP is a key ingredient to the accurate and timely forecast of weather elements. Its aim is to numerically predict future states of the atmosphere based on a current collection of data and an appropriate dynamic model. The dynamic core of NWP models consists of the classical Euler equations of fluid dynamics discretized in space and time. Both the spatial and temporal discretization aspects of NWP have been subject to intense research efforts over the years [1]. A particular problem in the time integration of the NWP model equations is that the maximum permissible time steps are governed by stability rather than accuracy considerations. This is due to the coexistence of several fluid regimes of which only the slowly varying ones are of atmospheric relevance. To circumvent the resulting severe restrictions on the achievable time steps, the following two strategies have been followed. Firstly, one can derive reduced NWP model equations, which explicitly filter out undesired fluid regimes. Secondly, one can apply semi-implicit or fractional time stepping methods to the unapproximated Euler equations [1]. Both strategies have been successfully applied to NWP. However, the dominant trend is towards the numerical integration of unapproximated fluid equations using semi-implicit or fractional time stepping methods. The semi-implicit semi-Lagrangian (SISL) method, as originally proposed by Robert [5], is among the most popular of those methods. The two essential ingredients are a linearly implicit treatment of fast waves and a semi-Lagrangian treatment of advection. In this paper, we suggest an alternative implementation of these two ideas. This new approach can be put into the framework of the Störmer-Verlet method [4], widely used in classical mechanics, and a regularization of the governing fluid equations as suggested by Frank, Gottwald & Reich [2] and further developed by Frank, Reich, Staniforth, White & Wood [3] and Wood, Staniforth & Reich [9]. Ultimately this new regularized Störmer-Verlet scheme is to be applied to the unapproximated 3D Euler equations. In this paper, however, we restrict the discussion to the 2D shallow-water equations (SWEs). These equations are often used in NWP to test new algorithmic ideas.

We wish to point out that an alternative semi-Lagrangian implementation of the regularized fluid equations has been proposed by Staniforth, Wood & Reich in [8].

2 Shallow-water equations

A 2D model of the atmosphere which retains the important dynamic interactions of real atmospheric flows is the orographically forced SWEs on an f-plane [1, 6]:

$$\frac{Du}{Dt} = +fv - g\mu_x - g\mu_x^S, \tag{2.1}$$

$$\frac{Dv}{Dt} = -fu - g\mu_y - g\mu_y^S, \tag{2.2}$$

$$\frac{D\ln\mu}{Dt} = -u_x - v_y. \tag{2.3}$$

Here $\mu^S = \mu^S(x,y)$ is the height of the orography above mean sea level and $\mu = \mu(x,y,t)$ is the fluid depth, i.e., the depth of the fluid between the orography and the fluid's free surface. Also, g is the gravitational constant, f is twice the (constant) angular velocity of the reference plane,

$$\frac{D}{Dt}(.) = (.)_t + u\,(.)_x + v\,(.)_y\,, \tag{2.4}$$

is the Lagrangian or material time derivative, and subscripts denote partial differentiation with respect to that variable.

The positions (x, y) of a material fluid particle are related to the velocity field (u, v) by the kinematic relation

$$\frac{Dx}{Dt} = u, \qquad \frac{Dy}{Dt} = v. \tag{2.5}$$

If, furthermore, we rewrite (2.1)-(2.2) in the form

$$\frac{Du}{Dt} = F^x, \qquad \frac{Dv}{Dt} = F^y \tag{2.6}$$

with the forces F^x and F^y determined by

$$F^x := +fv - g\mu_x - g\mu_x^S, \qquad F^y := -fu - g\mu_y - g\mu_y^S, \tag{2.7}$$

we conclude that equations (2.5) and (2.6) are reminiscent of those of classical mechanics with particles moving on a plane. The significant difference is that, in case of fluid dynamics, we are dealing with a continuum of particles and that the time evolution of (u, v, η) can be evaluated without use of the kinematic relations (2.5) by employing (2.4) instead. For historic reasons, the classical mechanics approach to fluid dynamics is called the Lagrangian description, while the formulation (2.1)-(2.3) together with (2.4) is called the Eulerian description. See SALMON [6] for more details.

A linearization of the equations (2.1)-(2.3) reveals that there are two basic kinds of associated motion, fast moving gravitational oscillations and slow moving Rossby waves. Geostrophic theory reveals furthermore that Rossby waves move to leading order with the local wind speed. Geostrophic theory is based on potential vorticity (PV) conservation, i.e.

$$\frac{Dq}{Dt} = 0, \qquad q = \frac{v_x - u_y + f}{\eta}, \tag{2.8}$$

and the geostrophic balance relations

$$0 \approx fv - g\mu_x - g\mu_x^S, \qquad 0 \approx -fu - g\mu_y - g\mu_y^S. \tag{2.9}$$

Note that (2.9) can be solved for the wind field (u, v) in case of strict equality, which can be used to approximately advect the PV field q using (2.8). Knowledge of the PV field on the other hand allows for the computation of a balanced fluid depth μ via a process called PV inversion. PV inversion turns equations (2.8)-(2.9) into a closed set of (filtered) equations for the approximate time evolution of Rossby waves. See SALMON [6] for further details.

When numerically solving the unapproximated SWEs (2.1)-(2.3), large scale Rossby waves should be resolved accurately while gravitational oscillations are of little or no significance for atmospheric flow regimes. This suggests to apply an implicit time stepping method to treat the insignificant gravitational oscillations and a semi-Lagrangian method to resolve the geostrophic advection processes to high accuracy. The most popular of these methods is the semi-implicit semi-Lagrangian (SISL) method of ROBERT, which we briefly describe next.

We wish to emphasize that this paper is entirely devoted to the issue of time-stepping. Spatial discretization aspects are largely ignored throughout the text.

3 Semi-implicit semi-Lagrangian method

The SISL method has been designed with the goal of being able to use large time steps, while not compromising on the accuracy in the advection of Rossby modes. We follow here the description of the method given by Staniforth & Coté [7].

We first introduce a few notations to shorten the presentation. In particular, we define the two vectors $\mathbf{x} = (x, y)^T$, $\mathbf{u} = (u, v)^T$,

$$\mathbf{F} = (F^x, F^y)^T = -f\mathbf{u}^\perp - g\nabla(\mu + \mu^S), \tag{3.1}$$

as well as $\mathbf{u}^\perp = (-v, u)^T$ and $\nabla = (\partial_x, \partial_y)^T$.

The definition of departure and arrival points is essential to the semi-Lagrangian method. We denote arrival points by $\mathbf{x}_a$. Arrival points are grid points while the departure points $\mathbf{x}_d^n$ at time-level t_n are computed using a discretization of the kinematic equations (2.5). We furthermore denote quantities approximated at departure points by subscript d, e.g. $\mathbf{u}_d^n$. These approximations are derived by interpolating known grid values, e.g. $\mathbf{u}^n$, to the departure point locations. See [1, 7] for details.

The first step to derive a semi-implicit semi-Lagrangian method is to formulate a fully implicit semi-Lagrangian method

$$\mathbf{u}^{n+1} = \mathbf{u}_d^n + \frac{\Delta t}{2}\left(\mathbf{F}^{n+1} + \mathbf{F}_d^n\right), \tag{3.2}$$

$$\ln \mu^{n+1} = [\ln \mu^n]_d - \frac{\Delta t}{2}\left([u_x + v_y]^{n+1} + [u_x + v_y]_d^n\right), \tag{3.3}$$

$$\mathbf{x}_a = \mathbf{x}_d^n + \frac{\Delta t}{2}\left(\mathbf{u}^{n+1} + \mathbf{u}_d^n\right). \tag{3.4}$$

This method is equivalent to a trapezoidal rule discretization of the Lagrangian description of fluid mechanics put within the context of semi-Lagrangian methods. A semi-implicit method is obtained by applying a linearly implicit predictor-corrector approximation to (3.2)-(3.3) and by replacing (3.4) with an explicit extrapolation formula. See [1, 7] for details. While these two modifications lead to efficiency gains, they also compromise on the accuracy and stability of the method. In particular, the semi-implicit method is no longer centered-in-time.

4 Regularized shallow-water equations

An alternative method to the integration of the SWEs has been proposed by Gottwald, Frank & Reich [2] in the context of the Hamiltonian particle-mesh (HPM) method. The HPM method is based on the Lagrangian description of fluid mechanics and a Störmer-Verlet time-stepping [4] of the form

$$\mathbf{u}^{n+1/2} = \mathbf{u}^n + \frac{\Delta t}{2}\mathbf{F}^n, \tag{4.1}$$

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t \mathbf{u}^{n+1/2}, \tag{4.2}$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{n+1/2} + \frac{\Delta t}{2}\mathbf{F}^{n+1}, \tag{4.3}$$

where

$$\mathbf{F}^n = -f(\mathbf{u}^n)^\perp - g\nabla(\mu^n + \mu^S) \tag{4.4}$$

and the correspondingly time shifted formulation for $\mathbf{F}^{n+1}$. The required fluid depth approximation μ^n can be derived from the particle distribution $\mathbf{x}^n$. See [2] for details.

Explicit time stepping methods, such as Störmer-Verlet, are subject to severe step size restrictions. To partially overcome those restrictions, it was suggested by Frank, Gottwald & Reich [2] to regularize the fluid depth μ by a smoothing operator

$$\mathcal{A} = \left[1 - \alpha^2\nabla^2\right]^{-1}. \tag{4.5}$$

and to replace the force (4.4) by the regularized expression

$$\mathbf{F}^n = -f(\mathbf{u}^n)^\perp - g\nabla(\mathcal{A} * \mu^n + \mu^S). \tag{4.6}$$

Besides allowing for larger time-steps the smoothing was also found to prevent the particle method from generating unbalanced gravity waves.

The analysis of Frank, Reich, Staniforth, White & Wood [3] resulted in an optimal choice for the parameter α in terms of linear stability. However, it was also found that (4.6) corrupts the geostrophic balance relation (2.9) of the unregularized equations with potentially harmful effects on the advection of Rossby waves.

In the subsequent publication [9], Wood, Staniforth & Reich suggested a refined regularization procedure. Define a regularized fluid depth $\tilde{\mu}^n$ by

$$\left[1 - \alpha^2\nabla^2\right](\tilde{\mu}^n - \mu^n) = \alpha^2\left[\frac{f}{g}(u_y^n - v_x^n) + \nabla^2(\mu^n + \mu^S)\right] \tag{4.7}$$

with the parameter α chosen as

$$\alpha^2 = \frac{gH\Delta t^2/4}{1 + f^2\Delta t^2/4}. \tag{4.8}$$

Here H denotes the maximum value of μ over the whole fluid domain. The regularized fluid depth $\tilde{\mu}^n$ replaces $\mathcal{A} * \mu^n$ in (4.6) to yield the improved formulation

$$\mathbf{F}^n = -f(\mathbf{u}^n)^\perp - g\nabla(\tilde{\mu}^n + \mu^S). \tag{4.9}$$

The resulting regularized Störmer-Verlet method is equivalent to the SISL method on the level of linearized equations and zero mean advection. See [9] for details. Furthermore $\tilde{\mu} = \mu$ in case of exact geostrophic balance, i.e., exact equality in (2.9).

5 Regularized semi-Lagrangian Störmer-Verlet method

We are now in a position to describe the newly proposed semi-Lagrangian implementation of the regularized Störmer-Verlet method.

Step 1 (half time step of Eulerian momentum update). We assume that (u^n, v^n), and the regularized $\tilde{\mu}^n$ are known. Update the velocities (u,v) over the given grid according to:

$$u^{n+1/2-\varepsilon} = u^n + \frac{\Delta t}{2}\left[f\, v^{n+1/2-\varepsilon} - g\,(\tilde{\mu}_x^n + \mu_x^S)\right], \tag{5.1}$$

$$v^{n+1/2-\varepsilon} = v^n - \frac{\Delta t}{2}\left[f\, u^{n+1/2-\varepsilon} + g\,(\tilde{\mu}_y^n + \mu_y^S)\right]. \tag{5.2}$$

We use superscript $-\varepsilon$ in $(u^{n+1/2-\varepsilon}, v^{n+1/2-\varepsilon})$ to indicate that these are the values of (u,v) just before the advection step. Similarly, we will use superscript $+\varepsilon$ to denote the values of (u,v) immediately after the advection step which we describe next.

Step 2 (full time step of force-free advection). This step gets split into two substeps. The first part determines the particle paths and the velocities are updated according to

$$\frac{Du}{Dt} = \frac{Dv}{Dt} = 0, \qquad \frac{Dx}{Dt} = u, \quad \frac{Dy}{Dt} = v. \tag{5.3}$$

The exact solutions are given by linear trajectories, which we approximate using

$$x_a = x_d^n + \Delta t\, u_d^{n+1/2-\varepsilon}, \tag{5.4}$$

$$y_a = y_d^n + \Delta t\, v_d^{n+1/2-\varepsilon}, \tag{5.5}$$

where $(u_d^{n+1/2-\varepsilon}, v_d^{n+1/2-\varepsilon})$ are obtained from the grid values $(u^{n+1/2-\varepsilon}, v^{n+1/2-\varepsilon})$ by bilinear interpolation to the departure points. The equations (5.4)-(5.5) are solved by simple fixed point iteration.

Once the fixed point iteration has converged, bicubic interpolation is used to first obtain $(u_d^{n+1/2-\varepsilon}, v_d^{n+1/2-\varepsilon})$ and, finally, the new updated values of $(u^{n+1/2+\varepsilon}, v^{n+1/2+\varepsilon})$ over the grid via

$$u^{n+1/2+\varepsilon} = u_d^{n+1/2-\varepsilon}, \qquad v^{n+1/2+\varepsilon} = v_d^{n+1/2-\varepsilon}. \tag{5.6}$$

Next we update the layer-depth μ^n according to the continuity equation (2.3). We apply the symmetric semi-Lagrangian formulation

$$\ln \mu^{n+1} + \frac{\Delta t}{2}\left[u_x + v_y\right]^{n+1/2+\varepsilon} = \left[\ln \mu^n - \frac{\Delta t}{2}\left(u_x^{n+1/2-\varepsilon} + v_y^{n+1/2-\varepsilon}\right)\right]_d. \tag{5.7}$$

The departure point approximation is done using bicubic interpolation with the departure points defined by (5.4)-(5.5).

Step 3 (half time step of Eulerian momentum update). We compute the new regularized fluid depth $\tilde{\mu}^{n+1}$ using

$$\left(1-\alpha^2\nabla^2\right)\tilde{\mu}^{n+1} = \mu^{n+1} - \alpha^2\frac{f_0}{g}\zeta^{n+1}, \tag{5.8}$$

where

$$\zeta^{n+1} = v_x^{n+1} - u_y^{n+1} \tag{5.9}$$

is the vorticity at time level t_{n+1}. The velocity update is explicitly defined by

$$u^{n+1} = u^{n+1/2+\varepsilon} + \frac{\Delta t}{2}\left[f\,v^{n+1/2+\varepsilon} - g\,(\tilde{\mu}_x^{n+1} + \mu_x^S)\right], \tag{5.10}$$

$$v^{n+1} = v^{n+1/2+\varepsilon} - \frac{\Delta t}{2}\left[f\,u^{n+1/2+\varepsilon} + g\,(\tilde{\mu}_y^{n+1} + \mu_y^S)\right]. \tag{5.11}$$

Note that the value of ζ^{n+1} does not depend on $\tilde{\mu}^{n+1}$ and that *Step 3* is hence entirely explicit except for the solution of a modified Helmholtz problem (5.8).

It can be shown that the scheme given by (5.1)-(5.11) is centered-in-time up to higher order asymmetries due to interpolation errors in the semi-Lagrangian advection under *Step 2*. Hence the method is second-order in time. Note that the semi-Lagrangian advection in *Step 2* could be replaced by other methods suitable for advection problems [1].

Following the linear analysis provided in [8] for a similar discretization, it can be shown that the newly proposed method is linearly equivalent to the SISL method not only under zero mean advection [9] but also in case of non-vanishing mean advection. This statement follows from the fact that (5.1)-(5.11) can be viewed as a composition method (see, for example, [4]) and the property that advection and wave propagation commute on a linearized equation level [1].

6 Numerical experiment

Both the fully implicit SL scheme (3.2)-(3.4) as well as the newly proposed semi-Lagrangian implementation of the regularized Störmer-Verlet method have been implemented using the standard C-grid [1] over a double periodic domain with $L_x = L_y = 3840$ km (see [8] for details). The grid size is $\Delta x = \Delta y = 60$ km. The time step is $\Delta t = 20$ min and the value of f corresponds to an f-plane at 45^o latitude. The reference height of the fluid is set to $H = 9665$ m. The resulting smoothing length (4.8) satisfies $\alpha \approx 3.3\,\Delta x$. The Rossby radius of deformation is $L_R \approx 3000$ km. The maximum initial wind speed is approximately 11 m s^{-1}.

In Fig. 6.1, we display the computed time evolution of potential vorticity (PV) over a time period of 6 days using the newly proposed semi-Lagrangian Störmer-Verlet (SLSV) method (5.1)-(5.11). We also provide the difference to the PV field obtained from the fully implicit semi-Lagrangian method (3.2)-(3.4). (The reference solution from the fully implicit semi-Lagrangian method can be found in [8].) The results indicate that the SLSV method and the fully implicit SL

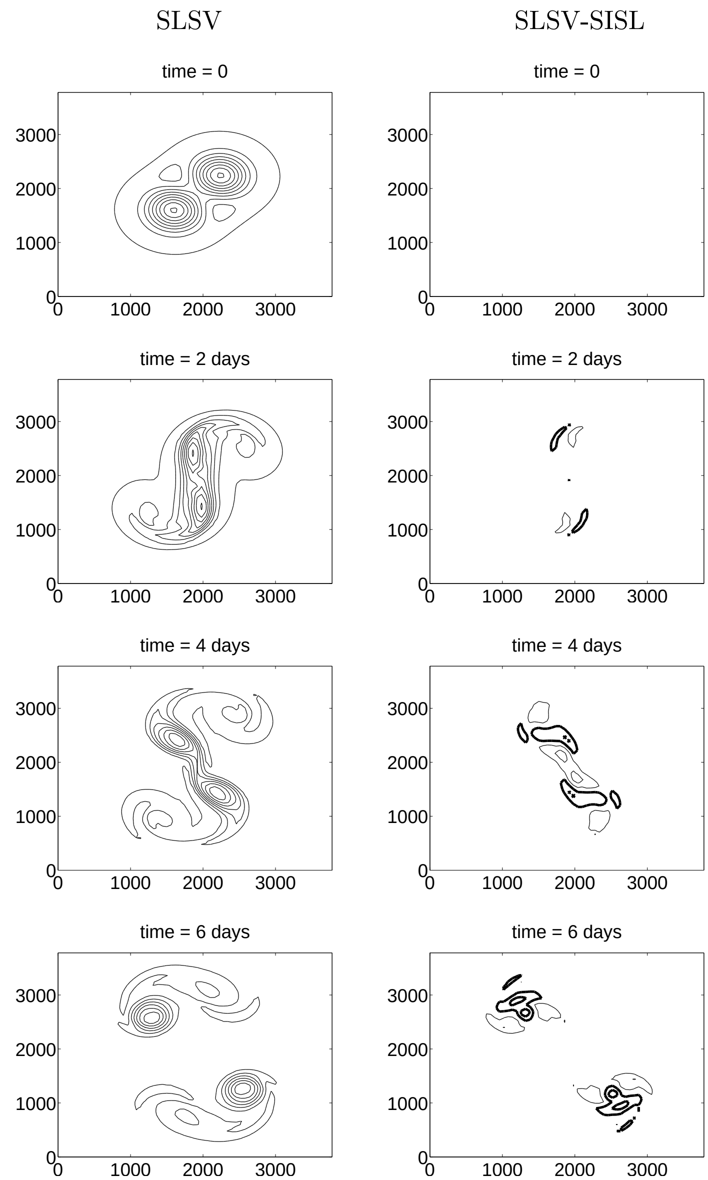

Figure 6.1: Left panels: Computed time evolution, from initial time to $t = 6$ days, of PV over the domain $(x, y) \in [0, 3840\,\mathrm{km}] \times [0, 3840\,\mathrm{km}]$ using the semi-Lagrangian Störmer-Verlet (SLSV) method with timestep $\Delta t = 20\,\mathrm{min}$. Contours plotted between $6.4 \times 10^{-8}\,\mathrm{m}^{-1}\mathrm{s}^{-1}$ and $2.2 \times 10^{-7}\,\mathrm{m}^{-1}\mathrm{s}^{-1}$ with contour interval $1.56 \times 10^{-8}\,\mathrm{m}^{-1}\mathrm{s}^{-1}$. Right panels: Differences (semi-Lagrangian Störmer-Verlet minus fully implicit semi-Lagrangian) at corresponding times are plotted with a 10 times smaller contour interval, where thin (thick) lines are positive (negative) contours.

method (3.2)-(3.4) lead to similar results for strongly nonlinear flow regimes (in addition to being equivalent on a linearized equation level). Finally, note that stability would require a time step of $\Delta t \approx 1.6$ min for a traditional explicit Eulerian leapfrog method [1].

7 Conclusion

We have presented a promising alternative to the popular SISL method. The new method shares the same linear stability properties as the SISL method and maintains geostrophic balance relations. It is based on a semi-Lagrangian and linearly implicit implementation of the popular Störmer-Verlet method applied to a set of regularized fluid equations. An alternative implementation has been proposed by Staniforth, Wood & Reich in [8].

Acknowledgments. We would like to thank Jason Frank, Andrew Staniforth, and Nigel Wood for discussions on the subject of this paper.

REFERENCES

1. D.R. Durran. *Numerical Methods for Wave Equations in Geophysical Fluid Dynamics*. Springer-Verlag, Berlin Heidelberg, 1998.
2. J. Frank, G. Gottwald, and S. Reich. The Hamiltonian particle-mesh method. In M. Griebel and M.A. Schweitzer, editors, *Meshfree Methods for Partial Differential Equations, Lecture Notes in Computational Science and Engineering*, volume 26, pages 131–142, Berlin Heidelberg, 2002. Springer-Verlag.
3. J. Frank, S. Reich, A. Staniforth, A. White, and N. Wood. Analysis of a regularized, time staggered discretization and its link to the semi-implicit method. *Atm. Sci. Lett.*, 6:97–104, 2005.
4. B. Leimkuhler and S. Reich. *Simulating Hamiltonian Dynamics*. Cambridge University Press, Cambridge, 2005.
5. A. Robert. A semi-Lagrangian and semi-implicit numerical integration scheme for the primitive meteorological equations. *Jpn. Meteor. Soc.*, 60:319–325, 1982.
6. R. Salmon. *Lectures on Geophysical Fluid Dynamics*. Oxford University Press, Oxford, 1999.
7. A. Staniforth and J. Coté. Semi-Lagrangian integration schemes for atmospheric models – A review. *Mon. Wea. Rev.*, 119:2206–2223, 1991.
8. A. Staniforth, N. Wood, and S. Reich. A time-staggered semi-Lagrangian discretization of the rotating shallow-water equations. *Q.J.R. Meteorolog. Soc.*, submitted, 2006.
9. N. Wood, A. Staniforth, and S. Reich. An improved regularization for time-staggered discretization and its link to the semi-implicit method. *Atm. Sci. Lett.*, 7:21–25, 2006.